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# Fast low-rank approximations of multidimensional integrals in ion-atomic collisions modelling

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SUMMARY

An efficient technique based on low-rank separated approximations is proposed for computation of three-dimensional integrals arising in the energy deposition model that describes ion-atomic collisions. Direct tensor-product quadrature requires grids of size $4000^3$ which is unacceptable. Moreover, several of such integrals have to be computed simultaneously for different values of parameters. To reduce the complexity, we use the structure of the integrand and apply numerical linear algebra techniques for the construction of low-rank approximation. The resulting algorithm is $10^3$ faster than spectral quadratures in spherical coordinates used in the original DEPOSIT code. The approach can be generalized to other multidimensional problems in physics. Copyright © 0000 John Wiley & Sons, Ltd.

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KEY WORDS: Low-rank approximation; 2D cross; Separated representation; Exponential sums; 3D Integration; Slater wave function

## 1. INTRODUCTION

Computation of multidimensional integrals is one of the most time-consuming tasks in physics. Standard approaches either have high complexity or require sophisticated quadrature schemes. Already in a three-dimensional case the integrand may depend on many parameters and should be computed many times, so the computational cost of the simplest tensor-product quadratures is an important issue.

One of the promising tools to reduce the dimensionality of the problem (and hence the number of mesh points where the integrand should be calculated) is the usage of *separation of variables* in the integrand (see, for example, [1, 2]). The idea was known for a long time (for examples we refer the reader to the review [3]), but it has become practically useful after the fast algorithms of decompositions of functions in a *separated form* had been obtained in two- [4, 5], three- [6, 7] and multidimensional cases [8, 9].

Let $F(x, y)$ be a function of two variables $x, y$ where point $(x, y)$ is in a certain rectangle $[a_x, b_x] \otimes [a_y, b_y]$. The function is said to be in a *separated form* if it can be represented as a sum of products of univariate functions:

$$F(x, y) = \sum_{\tau=1}^{q} \sigma_\tau \, u_\tau(x) g_\tau(y). \tag{1}$$

The minimal number $q$ such that (1) exists is called *separation rank*. Direct generalization of (1) to multivariate functions is referred to as a canonical polyadic (CP, also known as

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CANDECOMP/PARAFAC) decomposition [3, 10]. The reader can find examples of applications of separated representations in multidimensional cases in [1, 11, 12, 13, 14, 15, 16, 17, 18, 19].

For a function given in the separated form the integration is simplified a lot. Indeed,

$$\iint F(x,y)dxdy = \sum_{\tau=1}^{q} \sigma_\tau \int_{a_x}^{b_x} u_\tau(x)dx \int_{a_y}^{b_y} g_\tau(y)dy, \tag{2}$$

and the problem is reduced to the computation of one-dimensional integrals, which can be computed using fewer quadrature points than the original integral.

In case of a discrete approximation of (1)

$$F(x_i,y_j) \approx \sum_{\tau=1}^{q} \sigma_\tau u_\tau(x_i) g_\tau(y_j) \tag{3}$$

with the error $\varepsilon$ in the Frobenious norm the number $q$ is called $\varepsilon$-rank. We shall assume the notion of $\varepsilon$-rank when the term *rank* will be mentioned in the text bellow. Expression (3) can be rewritten in the matrix form

$$A \approx U\Sigma G^\top, \tag{4}$$

where $A$ is an $n \times m$ matrix with elements $A_{ij} = F(x_i, y_j)$, $U$ is an $n \times q$ matrix with elements $U_{i\tau} = u_\tau(x_i)$, $G$ is an $m \times q$ matrix with elements $G_{j\tau} = g_\tau(y_j)$ and $\Sigma$ is a $q \times q$ diagonal matrix with elements $\sigma_\tau$ on the diagonal. This is a standard *low-rank approximation problem* for a given matrix. Provided that a good low-rank approximation exists, there are very efficient *cross approximation algorithms* [4, 5] that need only $\mathcal{O}((n+m)q)$ elements of a matrix to be computed.

In this paper we describe how to apply this technique to speedup computations of three-dimensional integrals in the energy deposition model intended to describe ion-atomic collisions. This model was introduced by N. Bohr [20] and developed further by A. Russek and J. Meli [21], C.L. Cocke [22], and V.P. Shevelko *at al.* [23]. Theoretical development of the model is presented in [23, 24, 25, 26]. Examples of calculations are reported in [27, 28, 29, 30]. Detailed description of the computer code DEPOSIT and user guide are given in [31] and its updated version based on the separated representations is avialable in [32].

The code DEPOSIT allows to calculate total and multiple electron loss cross sections and ionization probabilities needed for estimation of losses and lifetimes of fast ion beams, background pressures and pumping requirements in accelerators and storage rings. All of them are, in fact, functionals of the deposited energy $T(b)$ ($b$ is the impact parameter of the projectile ion), which in turn is a three-dimensional integral over the coordinate space. To calculate any of these parameters one has to compute $T(b)$ in all points of the $b$-mesh.

In the original work [31] an advanced quadrature technique was used, and the computational time has appeared to be much faster in a comparison with direct usage of uniform meshes. Calculation of the deposited energy $T(b)$ for a given atomic shell in one point $b$ took about several seconds. For complex ions it was about few hours on one processor core in total, that is not enough fast. To overcome this issue a fully scalable parallel variant of the algorithm was proposed, but the computational time was still large.

We present an entirely different approach for the computation of $T(b)$ in many points of the $b$-mesh based on the idea of separation of variables (1). An approximation of functions to be integrated by a sum of products of univariate functions allows to effectively decrease the dimensionality of the problem. This requires active usage of numerical and analytical tools.

The problem setting is as follows. The deposited energy $T(b)$ is a three-dimensional integral

$$T(b) = \iiint \Delta E(x, z-b)\rho(x,y,z)dxdydz. \tag{5}$$

It involves cylindrically symmetric function of two variables (the energy gain $\Delta E$ during an ion-atomic collision) which is a smooth finite function and spherically symmetric function of three variables (electron density in a Slater-type approximation) which decays exponentially. For details



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and definitions we refer the reader to Appendix A. Previous approach [31] used tensor-product quadratures in spherical coordinates. We use very fine uniform meshes and low-rank approximation.

In Section 2.1 the Slater-type function of three variables is decomposed by the exponential sums approach [33, 34]. The integral is immediately reduced to a two-dimensional one of a simpler structure. In Section 2.2 for a function of two variables we use the pseudo-skeleton decomposition of matrices [35, 36, 37] computed via a variant of the incomplete cross approximation algorithm [4]. Combining these two representations we obtain then an efficient algorithm with $\mathcal{O}(n)$ scaling, in comparison with $\mathcal{O}(n^3)$ complexity for direct integration over a three-dimensional mesh. We show numerically that the function in question can be well-approximated by a separable function. Thus, the approximation can be computed in $\mathcal{O}(n)$ time, where $n$ is the number of grid points in one dimension. The computation of $T(b)$ on the whole $b$-mesh takes less then one minute instead of several hours and total speedup of the program is about $\sim 10^3$ times. Illustrative examples are given in Section 2.3. All the equations related to the physical model are written in atomic units.

## 2. NUMERICAL PROCEDURE

### *2.1. Exponential sums.*

In this section we present analytical expansion of the spherically symmetric electron density $\rho_\gamma(r)$ in Cartesian coordinates as a sum of separable functions. We use this decomposition later in Section 2.2 for analytical integration in one dimension.

A three-dimensional electron density $\rho_\gamma(r)$ is taken in a Slater-type approximation

$$\rho_\gamma(r) = C_\gamma r^{\alpha_\gamma} e^{-2\beta_\gamma r}, \qquad r = \sqrt{x^2+y^2+z^2}, \tag{6}$$

where integer parameter $\alpha_\gamma$ and real $C_\gamma$ and $\beta_\gamma$ correspond to one atomic shell labeled by $\gamma$ (see also Appendix B for description of parameters). For the density $\rho_\gamma(r)$ the following normalization condition occurs

$$\int_0^\infty \rho_\gamma(r)dr = N_\gamma, \tag{7}$$

where $N_\gamma$ is the number of electrons in a $\gamma$-shell. For the sake of simplicity index $\gamma$ will be skipped and only one shell will be considered in equations bellow.

For a function $\rho(x,y,z)$ defined in (6) the separation of variables (1) in Cartesian coordinates can be done analytically [33, 34, 38, 39]. The main idea is to approximate the Slater density function by a sum of Gaussians

$$\rho(r) \approx \sum_{k=0}^{K} \lambda_k e^{-\eta_k r^2}. \tag{8}$$

Once the approximation (8) is computed, the separation of variables in Cartesian coordinates is immediately done

$$\rho(x,y,z) \approx \sum_{k=0}^{K} \lambda_k \, e^{-\eta_k x^2} \, e^{-\eta_k y^2} e^{-\eta_k z^2}. \tag{9}$$

The technique for computation of nodes $\lambda_k$ and weights $\eta_k$ is based on the computation of inverse Laplace transform. Let us consider a function $f_{\alpha\beta}(t)$ such that its Laplace transform is a function $F_{\alpha\beta}(s)$:

$$F_{\alpha\beta}(s) = \frac{\rho(\sqrt{s}\,)}{C} = \left(\sqrt{s}\right)^\alpha e^{-2\beta\sqrt{s}} = \int_0^\infty e^{-st} f_{\alpha\beta}(t)\, dt, \tag{10}$$

where $\alpha$ and $\beta$ are parameters of Slater density (6). Inverse Laplace transform $f_{\alpha\beta}(x)$ can be computed analytically for known $F_{\alpha\beta}(s)$ (10). In Appendix B we present explicit expressions for functions $f_{\alpha\beta}(t)$ corresponding to function (10) for integer $\alpha$ and real positive $\beta$.



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Once function $f_{\alpha\beta}(t)$ in expression (10) is known, the integral (10) can be computed numerically and approximated by a quadrature formula

$$\rho(r) \approx C \sum_{k=0}^{K} w_k e^{t_k} f_{\alpha\beta}(e^{t_k}) e^{-r^2 e^{t_k}}. \tag{11}$$

Here $w_k$ and $e^{t_k}$ are quadrature weights and nodes, respectively. The procedure to compute weights and nodes was taken from the paper [34]. For the reader's convenience we give the formula and its derivation in Appendix C.

Comparision with equation (8) gives

$$\lambda_k = C\, w_k e^{t_k} f_{\alpha\beta}(e^{t_k}), \qquad \eta_k = e^{t_k}. \tag{12}$$

It appears that not many quadrature points (at fixed $r$) are required to achieve the accuracy of the expansion of order $10^{-7}$ in the Chebyshev norm due to the hyper-exponential decay. Practically, such an accuracy is quite enough for the physical meaning of the model. However, $r$ is going to be very small, as soon as the finer grids (i.e. for a large number of nodes) are required for higher precision. Estimation of upper bound $K$ in sum (11) which has the logarithmic dependence is given in Appendix D.

### *2.2. Fast computation of* $T(b)$.

In this section we describe a numerical scheme based on the cross decomposition of two dimensional integrand. Dimensionality reduction (from three to two dimensions) is achieved by means of the separated representation of Slater density obtained in the previous Section.

Discretization of one-dimensional integrals in (2) by some quadrature formula with nodes $x_i \in [a_x, b_x]$, $i = 1, \ldots, n$, $y_j \in [a_y, b_y]$, $j = 1, \ldots, m$ and weights $w_i^{(x)}$, $w_j^{(y)}$, leads to the approximation

$$\iint F(x,y)dxdy \approx \sum_{\tau=1}^{q} \sigma_\tau \sum_{i=1}^{n} w_i^{(x)} u_\tau(x_i) \sum_{j=1}^{m} w_j^{(y)} g_\tau(y_j). \tag{13}$$

To get the decomposition (3) we apply *2d-cross* algorithm [4, 40] implemented in [32].

A three-dimensional integral $T(b)$ defined in (5) can be reduced to a two-dimensional integral by means of the decomposition (9)

$$T(b) = \sum_{k=0}^{K} \lambda_k \iiint \Delta E(x, z-b)\, e^{-\eta_k x^2} e^{-\eta_k y^2} e^{-\eta_k z^2} dxdydz \tag{14}$$

and analytical evaluation of one-dimensional Gaussian integral

$$\int_{-\infty}^{\infty} e^{-\eta\, y^2} dy = \sqrt{\frac{\pi}{\eta}}, \tag{15}$$

$$T(b) = \sqrt{\pi} \sum_{k=0}^{K} \frac{\lambda_k}{\sqrt{\eta_k}} \iint \Delta E(x, z-b)\, e^{-\eta_k x^2} e^{-\eta_k z^2} dxdz. \tag{16}$$

Suppose that $\Delta E(x, z-b)$ has been decomposed as follows

$$\Delta E(x, z-b) \approx \sum_{\tau=1}^{q} \sigma_\tau u_\tau(x) g_\tau(z-b). \tag{17}$$

Then the integration (16) can be reduced to a sequence of one-dimensional integrations.

$$T(b) = \sqrt{\pi} \sum_{k=0}^{K} \frac{\lambda_k}{\sqrt{\eta_k}} \sum_{\tau=1}^{q} \sigma_\tau I_{\tau k} J_{\tau k}(b), \tag{18}$$



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$$I_{\tau k} = \int_{a_x}^{b_x} u_\tau(x) e^{-\eta_k x^2} dx, \tag{19}$$

$$J_{\tau k}(b) = \int_{a_y}^{b_y} g_\tau(z-b) e^{-\eta_k z^2} dz. \tag{20}$$

For the numerical approximation of integrals (19) and (20) we use quadrature formula with uniform quadrature nodes (although any suitable quadrature can be used)

$$I_{\tau k} = \sum_{i \,\in\, \Omega_\epsilon^x(k)} w_i^{(x)} u_\tau(x_i) e^{-\eta_k x_i^2}, \qquad \Omega_\epsilon^x(k) = \{\, i \mid e^{-\eta_k x_i^2} > \epsilon \,\} \tag{21}$$

$$x_i = -a_x + i\, h_x, \qquad 0 \le i \le 2N_x, \qquad h_x = a_x/N_x, \tag{22}$$

$$J_{\tau k}(b) = \sum_j w_j^{(z)}\, g_\tau(z_j - b) e^{-\eta_k z_j^2}, \tag{23}$$

$$z_j = -a_z + j\, h_z, \qquad 0 \le j \le 2N_z, \qquad h_z = a_z/N_z. \tag{24}$$

We sample the impact parameter $b$ (which can take only positive values) with the *same step* $h_z$

$$b_l = l\, h_z, \qquad 0 \le l \le N_z. \tag{25}$$

This allows us to introduce a new variable $\tilde{z} = z - b$ discretized as follows

$$\tilde{z}_k = -2a_z + k\, h_z, \qquad 0 \le k \le 3N_z, \tag{26}$$

and such that for the boundary conditions (24), (25), (26)

$$z_j - b_l = \tilde{z}_{j-l+N_z}. \tag{27}$$

Thus, the approximation problem (17) reduces to the low-rank approximation of the extended $(2N_x+1) \times (3N_z+1)$ matrix

$$\Delta E(x_i, \tilde{z}_j) = \sum_{\tau=1}^{r} \sigma_\tau u_\tau(x_i) g_\tau(\tilde{z}_j). \tag{28}$$

This should be done only once (using the cross approximation algorithm), and the final approximation of integral (23) reads

$$J_{\tau k}(b_l) = \sum_{j \,\in\, \Omega_\epsilon^{\tilde{z}}(k)} w_j^{(\tilde{z})}\, g_\tau(\tilde{z}_{j-l+N_z}) e^{-\eta_k \tilde{z}_j^2}. \tag{29}$$

The calculation of $T(b)$ can be summarized in the following algorithm.

**for** every $\gamma$-shell of the projectile ion **do**
  compute the decomposition (8) for $\rho(r)$
  compute the cross approximation for the matrix $\Delta E(x_i, \tilde{z}_j)$ defined in (28)
  **for** $k = 0 \ldots K$ **do**
    **for** $\tau = 1 \ldots q$ **do**
      compute the integral $I_{\tau k}$ defined in (21)
  **for** every $b_l$ required **do**
    **for** $k = 0 \ldots K$ **do**
      **for** $\tau = 1 \ldots q$ **do**
        compute the integral $J_{\tau k}(b_l)$ defined in (29)
    compute $T_\gamma(b_l)$, equation (18)



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Finally, the question is how to compute $T(b)$ for many different values of $b$. The direct summation requires $\mathcal{O}(N^2)$ operations. But a closer look reveals that it is in fact a discrete convolution, which can be computed in linear cost. Nevertheless, due to the exponential decay of factors $e^{\eta_k x_i}$ and $e^{\eta_k \tilde{z}_j}$ in sums (21) and (29) correspondingly, there is a very small number of terms, such that a direct summation after the truncation is much faster. This can be easily seen from values of parameter $\theta_x$ defined as

$$\theta_x = \frac{\sum_{k=0}^{K} \mathcal{N}(\Omega_\epsilon^x(k))}{(2N_x+1)(K+1)}, \tag{30}$$

where $\mathcal{N}(X)$ is the cardinality of set $X$. For details, please, see Table II and discussion in the following Section 2.3.

### *2.3. Numerical experiments and discussions.*

Once the analytical expansion (9) is obtained, the full calculation of $T(b)$ consists of two steps (see algorithm in Section 2.2): calculation of the cross decomposition of integrand (16) on the extended $\tilde{z}$-mesh (26) and computation of all integrals $I_{\tau k}$ and $J_{\tau k}(b_l)$ for all $b_l$ from (25). There is no need in all the time recalculation of the cross approximation (28) for the full computation of these integrals. After it is computed (that is $\sigma_\tau$, $u_\tau(x_i)$ and $g_\tau(\tilde{z}_j)$ are known), the calculation of $I_{\tau k}$ and $J_{\tau k}(b_l)$ starts.

In Table I we present times $T_{\text{cross}}$ and ranks $q$ calculated for the energy gains $\Delta E_\gamma(x, \tilde{z})$ corresponding to two ion-atomic collision examples ($Au^{26+} + O$ and $U^{28+} + Xe$). Values of $T_{\text{cross}}$ are reported for different sizes of $(x, \tilde{z})$-mesh and the relative accuracy of the cross decomposition. One can find that $T_{\text{cross}}$ is about $10^{-1} \sim 10^0$ second in order of magnitude. Given that the full computation of integrals $I_{\tau k}$ and $J_{\tau k}(b_l)$ for all $b_l$ takes approximately $5000 \cdot 5 \cdot 10^{-3} = 25$ seconds (the average value of column $T_S$ in Table II for $5000$ $b$ values), we can conclude that the cross approximation becomes then a pre-computing stage with a tiny contribution to the total computational time.

An important parameter in sum (28) is the rank value $q$. It determines the complexity of the algorithm (the smaller $q$, the better). As it follows from the numerical experiments, ranks of $\Delta E_\gamma(x, \tilde{z})$ decomposition are small (Table I) against the mesh size. It means that for real physical systems the cross decomposition is a very prominent tool. It allows to decrease the complexity of the problem in practice from $O(n^2)$ elements to $O(q \cdot n)$ elements where $q \ll n$.

In Table II we present the program speedup for every atomic shell. In quadrature sum (21) all terms less then $\epsilon = 10^{-20}$ were thrown out for every $x_i$ due to the exponential decay of factors $e^{-\eta_k x_i^2}$ for every fixed $\eta_k$. Parameter $\theta_x$ is defined as a relative number of terms in total summation of $I_{\tau k}$ over all $k$ and $i$ (equation (21) and (30)), above the threshold $\epsilon$. As it can be seen from the table, there are only a few percent of terms to be summed, which considerably reduces the sum and speeds up the total calculation. Parameter $\theta_x$ decreases when going from top to bottom of the third column (for one system). That is why the time $T_S$ also decreases while both ranks $K$ and $q$ increase. The same situation occurs for sum (29) over $\tilde{z}_j$.

Another important question is the full accuracy of the computation. As it was mentioned above, it consists of two contributions acquired from the cross approximation and the quadrature summations. In equations (21) and (29) values $\sigma_\tau$, $u_\tau(x_i)$ and $g_\tau(\tilde{z}_j)$ are approximated with the cross accuracy $\varepsilon_c$, while the quadrature sum is calculated with an error $\varepsilon_i$. In Table III and Table IV we provide a numerical example demonstrating the actual error for the integral $T(b)$ for small enough mesh sizes. We consider the worst case $b = 0$, when the integrand has the most singular behavior (because the Slater density has no higher derivatives at $r = 0$). As it follows from our results the scheme holds the third order for the Simpson rule, even in the worst singular case. In other cases $b > 0$ it holds the fourth order. These results show that the claimed accuracy is achieved and the numerical scheme holds the order of integration up to the accuracy of the approximated function.

Finally, we can conclude that usage of the technique based on separated representations (18) allows to decrease the total time of computing of $T(b)$ by a factor of $\sim 10^3$ in comparison to the previous version. In practice, computational time is reduced from several hours to one minute or less on the same hardware.




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Table I. Ranks $q$ of the decomposition (28) calculated by incomplete cross approximation algorithm [4] for the energy gain $\Delta E(x, \tilde{z})$. Two cases are considered: collision of $Au^{26+}$ ions with an Oxigen atom at a collision energy $E = 6.5$ MeV/u and collision of $U^{28+}$ ions with a Xenon atom at a collision energy $E = 2.5$ MeV/u. The number of $x$-mesh points are taken equal to $2N + 1$, the number of $\tilde{z}$-mesh points is taken equal to $3N + 1$ in correspondence to equations (22) and (26), $a_x = a_z = 8$. The relative error of the approximation in the Frobenius norm $\varepsilon$ and $N$ are placed in the bottom line as a couple $(\varepsilon, N)$. They correspond to different numerical tests. Calculations were carried out on 1.3 GHz Intel Core i5 processor. Column $T_{\text{cross}}$ corresponds to the time the cross algorithm takes. The numerical results confirm almost linear scaling of the approach in $N$.

| System | $\gamma$-Shell | $q$ | $T_{\text{cross}}$ (sec) | $q$ | $T_{\text{cross}}$ (sec) | $q$ | $T_{\text{cross}}$ (sec) |
|---|---|---|---|---|---|---|---|
| $Au^{26+} + O$ | $4df^{17}$ | 13 | 0.21 | 21 | 0.42 | 24 | 2.41 |
| | $4sp^8$ | 13 | 0.21 | 21 | 0.33 | 24 | 2.40 |
| | $3d^{10}$ | 14 | 0.19 | 22 | 0.42 | 26 | 2.58 |
| | $3sp^8$ | 16 | 0.25 | 24 | 0.54 | 29 | 2.64 |
| | $2sp^8$ | 17 | 0.28 | 25 | 0.56 | 30 | 2.71 |
| | $1sp^2$ | 17 | 0.27 | 25 | 0.56 | 30 | 2.70 |
| $U^{28+} + Xe$ | $5sp^4$ | 14 | 0.20 | 22 | 0.50 | 26 | 2.17 |
| | $4df^{24}$ | 15 | 0.23 | 24 | 0.52 | 27 | 2.58 |
| | $4sp^8$ | 17 | 0.28 | 25 | 0.55 | 30 | 2.69 |
| | $3d^{10}$ | 17 | 0.27 | 25 | 0.54 | 30 | 2.77 |
| | $3sp^8$ | 17 | 0.27 | 25 | 0.55 | 30 | 2.75 |
| | $2sp^8$ | 17 | 0.26 | 25 | 0.54 | 30 | 2.71 |
| | $1sp^2$ | 17 | 0.26 | 25 | 0.55 | 30 | 2.69 |
| | | $(10^{-6}, 1024)$ | | $(10^{-9}, 1024)$ | | $(10^{-9}, 4096)$ | |

These results were obtained by using of our implementation of the cross approximation algorithm and the low-rank format of the Slater density (11). The latest version of the cross decomposition code implemented in $C$++ can be downloaded from the link [40].

## 3. CONCLUSIONS AND FUTURE WORK

A new and efficient technique for computation of three-dimensional integrals based on low-rank and separated representations is proposed for the energy deposition model. Due to a general form of the integrand, which is a product of two functions with cylindrical and spherical symmetries, this methodology can be applied to many types of integrals having similar structure. Such an approach significantly reduces computational time and allows to achieve a given accuracy (because it uses the cross approximation and quadrature summations). The general concept can be applied to more complicated models (like ion-molecular collisions with electron loss and charge-changing processes) that lead to multidimensional integrals. For the multidimensional case we plan to use fast approximation techniques based on the tensor train (TT) format [9].

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## A. PHYSICAL MODEL

In this section we introduce functions and parameters involved into the definition of deposited energy integral (5)

$$T_\gamma(b) = \iiint \Delta E_\gamma(p)\rho_\gamma(x, y, z)dxdydz, \tag{31}$$



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Table II. Timings to compute $T(b)$ at fixed $b$ are presented for two cases: the DEPOSIT code (old) $T_D$ and the code based on separated representations (18) $T_S$. Collision systems are the same as in Table I. In the third column $K$ labeles maximum value of index in expansion (9). The mesh (54) for radial density is taken with $a_t = -3$, $b_t = 45$, $h_t = (b_t - a_t)/250$. The meaning of parameter $\theta_x$ is explained in Section 2.3. Calculations were carried out for the relative accuracy of the cross decomposition $\varepsilon = 10^{-7}$ and $[-8, 8] \otimes [-16, 8]$ mesh with $4097 \times 6145$ points. The last column shows speedup of the program.

| System | $\gamma$-Shell | $K$ | $\theta_x \times 10^{-2}$ | $T_S$ ($\times 10^{-3}$ sec) | $T_D$ (sec) | $T_D/T_S$ |
|---|---|---|---|---|---|---|
| $Au^{26+} + O$ | $4df^{17}$ | 74 | 9.1 | 7.94 | 3.89 | 490 |
| | $4sp^8$ | 69 | 6.0 | 4.92 | 3.83 | 778 |
| | $3d^{10}$ | 73 | 4.3 | 3.59 | 3.88 | 1080 |
| | $3sp^8$ | 72 | 3.9 | 3.81 | 3.82 | 1003 |
| | $2sp^8$ | 107 | 1.5 | 2.42 | 3.86 | 1592 |
| | $1sp^2$ | 209 | 0.4 | 1.24 | 3.88 | 3120 |
| $U^{28+} + Xe$ | $5sp^4$ | 62 | 13.1 | 10.1 | 3.94 | 390 |
| | $4df^{24}$ | 70 | 6.5 | 6.05 | 3.90 | 644 |
| | $4sp^8$ | 67 | 5.1 | 5.00 | 3.94 | 788 |
| | $3d^{10}$ | 71 | 3.6 | 3.88 | 3.92 | 1011 |
| | $3sp^8$ | 70 | 3.4 | 3.52 | 3.90 | 1106 |
| | $2sp^8$ | 105 | 1.3 | 1.99 | 3.87 | 1945 |
| | $1sp^2$ | 207 | 0.3 | 1.04 | 3.88 | 3723 |

Table III. Convergence of integrals $T(b)$ for $4df^{17}$, $4sp^8$ and $3d^{10}$ shells of $Au^{26+} + O$ at 6.5 MeV/u on two-dimensional mesh $[-10, 10] \otimes [-20, 10]$ with $(2N + 1) \times (3N + 1)$ points for different $N$ (first column), see equations (22) and (26). Simpson weights $w_i^x$, $w_j^{(\bar{z})}$ are used in (21) and (29). For radial density the mesh (54) is taken with parameters $a_t = -3$, $b_t = 45$, $h_t = (b_t - a_t)/650$. Calculations were carried out for the relative accuracy of the cross decomposition $\varepsilon_c = 10^{-12}$ and fixed value of parameter $b_0 = 0.0$. Last column shows the rellative error $\varepsilon_i$. Extrapolated value of integral is calculated by Romberg method (with Richardson extrapolation) [41], p. 161. The order of scheme $p_e$ is defined by Aitken rule [41], p. 344.

| $\gamma$-Shell | $N$ | $q$ | $T(b_0)$ | $p_e$ | $\varepsilon_i$ |
|---|---|---|---|---|---|
| $4df^{17}$ | 2048 | 30 | 177.131769802401 | | $2.1 \cdot 10^{-7}$ |
| | 4096 | 33 | 177.131804304375 | | $1.2 \cdot 10^{-8}$ |
| | 8192 | 35 | 177.131806364504 | 4.07 | $7.7 \cdot 10^{-10}$ |
| | 16384 | 37 | 177.131806491972 | 4.01 | $4.8 \cdot 10^{-11}$ |
| | 32768 | 39 | 177.131806499918 | 4.00 | $3.0 \cdot 10^{-12}$ |
| | 65536 | 40 | 177.131806500407 | 4.02 | $2.3 \cdot 10^{-13}$ |
| | *extrapolated* | | 177.131806500448 | | |
| $4sp^8$ | 2048 | 31 | 165.507815905465 | | $2.2 \cdot 10^{-7}$ |
| | 4096 | 33 | 165.507850781567 | | $1.3 \cdot 10^{-8}$ |
| | 8192 | 35 | 165.507852865842 | 4.06 | $8.3 \cdot 10^{-10}$ |
| | 16384 | 37 | 165.507852994821 | 4.01 | $5.2 \cdot 10^{-11}$ |
| | 32768 | 39 | 165.507853002863 | 4.00 | $3.2 \cdot 10^{-12}$ |
| | 65536 | 40 | 165.507853003364 | 4.01 | $2.1 \cdot 10^{-13}$ |
| | *extrapolated* | | 165.507853003399 | | |
| $3d^{10}$ | 2048 | 33 | 407.589200892012 | | $5.0 \cdot 10^{-7}$ |
| | 4096 | 35 | 407.589382823491 | | $5.2 \cdot 10^{-8}$ |
| | 8192 | 38 | 407.589401536350 | 3.28 | $5.8 \cdot 10^{-9}$ |
| | 16384 | 40 | 407.589403612947 | 3.17 | $6.7 \cdot 10^{-10}$ |
| | 32768 | 42 | 407.589403853285 | 3.11 | $8.0 \cdot 10^{-11}$ |
| | 65536 | 44 | 407.589403882005 | 3.06 | $9.8 \cdot 10^{-12}$ |
| | 131072 | 46 | 407.589403885498 | 3.04 | $1.2 \cdot 10^{-12}$ |
| | 262144 | 47 | 407.589403885925 | 3.03 | $1.9 \cdot 10^{-13}$ |
| | *extrapolated* | | 407.589403886002 | | |



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Table IV. Convergence of integrals $T(b)$ for $3sp^8$, $2sp^8$ and $1s^2$ shells of $Au^{26+} + O$ at 6.5 MeV/u on two-dimensional mesh $[-10, 10] \otimes [-20, 10]$ with $(2N + 1) \times (3N + 1)$ points for different $N$ (first column), see equations (22) and (26). Simpson weights $w_i^x$, $w_j^{(\tilde{z})}$ are used in (21) and (29). For radial density the mesh (54) is taken with parameters $a_t = -3$, $b_t = 45$, $h_t = (b_t - a_t)/650$. Calculations were carried out for the relative accuracy of the cross decomposition $\varepsilon_c = 10^{-12}$ and fixed value of parameter $b_0 = 0.0$. Last column shows the rellative error $\varepsilon_i$. Extrapolated value of integral is calculated by Romberg method (with Richardson extrapolation) [41], p. 161. The order of scheme $p_e$ is defined by Aitken rule [41], p. 344.

| $\gamma$-Shell | $N$ | $q$ | $T(b_0)$ | $p_e$ | $\varepsilon_i$ |
|---|---|---|---|---|---|
| $3sp^8$ | 2048 | 35 | 53.0906497215656 | | $3.0 \cdot 10^{-5}$ |
| | 4096 | 38 | 53.0920135580097 | | $4.6 \cdot 10^{-6}$ |
| | 8192 | 41 | 53.0922247714446 | 2.69 | $6.1 \cdot 10^{-7}$ |
| | 16384 | 44 | 53.0922529097596 | 2.91 | $7.7 \cdot 10^{-8}$ |
| | 32768 | 47 | 53.0922564862273 | 2.98 | $9.7 \cdot 10^{-9}$ |
| | 65536 | 50 | 53.0922569351057 | 2.99 | $1.2 \cdot 10^{-9}$ |
| | 131072 | 52 | 53.0922569912665 | 3.00 | $1.5 \cdot 10^{-10}$ |
| | 262144 | 54 | 53.0922569982873 | 3.00 | $1.9 \cdot 10^{-11}$ |
| | 524288 | 56 | 53.0922569991611 | 3.01 | $2.4 \cdot 10^{-12}$ |
| | 1048576 | 58 | 53.0922569992692 | 3.01 | $4.0 \cdot 10^{-13}$ |
| | *extrapolated* | | 53.0922569992903 | | |
| $2sp^8$ | 2048 | 36 | 4.97891259072213 | | $2.3 \cdot 10^{-4}$ |
| | 4096 | 39 | 4.97986325621640 | | $3.5 \cdot 10^{-5}$ |
| | 8192 | 42 | 4.98001545713255 | 2.64 | $4.7 \cdot 10^{-6}$ |
| | 16384 | 45 | 4.98003568931593 | 2.91 | $5.9 \cdot 10^{-7}$ |
| | 32768 | 48 | 4.98003825660591 | 2.98 | $7.4 \cdot 10^{-8}$ |
| | 65536 | 51 | 4.98003857868963 | 2.99 | $9.2 \cdot 10^{-9}$ |
| | 131072 | 53 | 4.98003861898554 | 3.00 | $1.2 \cdot 10^{-9}$ |
| | 262144 | 56 | 4.98003862402352 | 3.00 | $1.4 \cdot 10^{-10}$ |
| | 524288 | 58 | 4.98003862465325 | 3.00 | $1.8 \cdot 10^{-11}$ |
| | 1048576 | 60 | 4.98003862473183 | 3.00 | $2.3 \cdot 10^{-12}$ |
| | 2097152 | 61 | 4.98003862474152 | 3.02 | $3.5 \cdot 10^{-13}$ |
| | *extrapolated* | | 4.98003862474327 | | |
| $1sp^2$ | 2048 | 36 | 0.122305706797573 | | $8.3 \cdot 10^{-3}$ |
| | 4096 | 39 | 0.123229108221677 | | $8.3 \cdot 10^{-4}$ |
| | 8192 | 42 | 0.123322068141309 | 3.31 | $7.9 \cdot 10^{-5}$ |
| | 16384 | 45 | 0.123330850494328 | 3.40 | $8.2 \cdot 10^{-6}$ |
| | 32768 | 48 | 0.123331746174083 | 3.29 | $9.1 \cdot 10^{-7}$ |
| | 65536 | 51 | 0.123331845477160 | 3.17 | $1.1 \cdot 10^{-7}$ |
| | 131072 | 53 | 0.123331857117543 | 3.09 | $1.3 \cdot 10^{-8}$ |
| | 262144 | 56 | 0.123331858525395 | 3.05 | $1.6 \cdot 10^{-9}$ |
| | 524288 | 58 | 0.123331858698474 | 3.02 | $2.0 \cdot 10^{-10}$ |
| | 1048576 | 59 | 0.123331858719929 | 3.01 | $2.5 \cdot 10^{-11}$ |
| | 2097152 | 61 | 0.123331858722600 | 3.01 | $3.1 \cdot 10^{-12}$ |
| | *extrapolated* | | 0.123331858722980 | | |

$$p = \sqrt{(z-b)^2 + x^2}, \tag{32}$$

where the integration is done over the whole coordinate space. Integral (31) is written for an atomic shell with *principal* quantum number $n$ and *orbital* quantum number $l$ labeled by $\gamma = nl$.

The energy gain $\Delta E_\gamma(p)$ is a kinetic energy deposited to the projectile's $\gamma$-shell by the field $U(R)$ of the target atom.

$$\Delta E_\gamma(p) = \Delta E_\gamma^<(p)\, n_f(v_\gamma - \vartheta) + \Delta E_\gamma^>(p)\, n_f(\vartheta - v_\gamma), \tag{33}$$

$$n_f(x) = \frac{1}{e^{-kx} + 1}, \tag{34}$$



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where $k = 3$ by default and is an input parameter of the model. Expression (33) consists of two terms corresponding to low

$$\Delta E_\gamma^<(p) = \frac{\xi_\gamma}{p + \zeta_\gamma} \sum_{i=1}^{3} \phi_i F(\chi_i p) \tag{35}$$

and high

$$\Delta E_\gamma^>(p) = \frac{\nu_\gamma}{p^2 + \mu_\gamma} \left( \sum_{i=1}^{3} \phi_i F(\chi_i p) \right)^2, \tag{36}$$

energies. Function

$$F(x) = xK_1(x) = \int_0^\infty e^{-\sqrt{x^2+y^2}} dy \tag{37}$$

is defined in terms of the *modified Bessel function of the second kind* $K_1(x)$ (see [42], p. 375, Eq. 9.6.2) with asympthotical behavior ([42], p. 378, Eq. 9.8.3 and p. 379, Eq. 9.8.7)

$$F(x \to 0_+) = 1 + \left( \frac{1}{2} \ln \frac{x}{2} + 0.03860786 \right) x^2 + \mathcal{O}(x^3). \tag{38}$$

Fitting parameters $\phi_i$, $\chi_i$ of the atomic field $U(R)$ are obtained from the Dirac-Hartree-Fock-Slater calculations [43]. The distance between the center of the field and the projectile electron of $\gamma$-shell is labeled by $R$. Atomic field is given in the Yukawa potential form

$$U(R) = -\frac{Z}{R} \sum_{i=1}^{3} \phi_i e^{-\chi_i R}, \tag{39}$$

where $Z$ is the nuclear charge of the target atom.

Parameter $\vartheta$ is a relative velocity of the projectile. It is related with the collision energy of the ion-atomic system. The rest parameters $v_\gamma$, $\xi_\gamma$, $\zeta_\gamma$, $\nu_\gamma$ and $\mu_\gamma$ concern to fundamental properties of the projectile ion and the target atom (such as binding energy, average velocity, mean radius of the shell, atomic radius and charge). They should be considered as positive constants in the integral (31) for a given ion-atomic system for all $b$. Detailed description of how to calculate them can be found in [31]. Examples of input files with the original code can be downloaded from link [44].

## B. INVERSE LAPLACE TRANSFORM SOURCES

For integer $\alpha$ and real positive $\beta$ inverse Laplace transform $f_{\alpha\beta}(t)$ of $F_{\alpha\beta}(s)$ from equation (10) may be calculated analytically and expressed via *the Kummer's confluent hypergeometric function* $M(a, b; z)$ ([42], chapter 13) as follows

$$f_{\alpha\beta}(t) = \frac{M\left(1 + \frac{\alpha}{2}, \frac{1}{2}, -\frac{\beta^2}{t}\right)}{t^{1+\frac{\alpha}{2}} \Gamma\left(-\frac{\alpha}{2}\right)} - 2\,\beta\, \frac{M\left(\frac{3+\alpha}{2}, \frac{3}{2}, -\frac{\beta^2}{t}\right)}{t^{\frac{3+\alpha}{2}} \Gamma\left(-\frac{1+\alpha}{2}\right)}, \tag{40}$$

where

$$M(a, b; z) = 1 + \frac{a}{b}\frac{z}{1!} + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \ldots \tag{41}$$

and $\Gamma(x)$ is *the Gamma function.*

Below we present $f_{\alpha\beta}(t)$ explicitly for most practically usefull cases ($\alpha = 0, 1, \ldots, 6$). Due to the difference of normalization conditions in spherical and Cartesian coordinates for the Slater density (6)

$$\rho(r) = N_\gamma \frac{(2\beta)^{2\mu+1}}{\Gamma(2\mu+1)} r^{2\mu} e^{-2\beta r}, \tag{42}$$

parameter $\alpha$ in (6) is related to parameter $\mu$ in (42) as follows

$$\alpha = 2\mu - 2. \tag{43}$$

The number of electrons in the shell $\gamma$ is labeled as $N_\gamma$. Parameter $\mu$ is greater or equal to unity. It is an integer or half-integer depending on *the principal quantum number* $n$ and *the orbital quantum number* $l$




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of the atomic shell. Details can be found in [45, 46]. For example, $\mu_{1s^2} = 1$, $\alpha = 0$; $\mu_{2sp^8} = 2$, $\alpha = 2$; $\mu_{4d^{10}} = 3.5$, $\alpha = 5$. Finally,

$$f_{0\beta}(t) = \frac{g_0\left(t/\beta^2\right)}{\sqrt{\pi}\,\beta^2}, \quad g_0(t) = \frac{e^{-\frac{1}{t}}}{t^{3/2}} \tag{44}$$

$$f_{1\beta}(t) = \frac{g_1\left(t/\beta^2\right)}{2\sqrt{\pi}\,\beta^3}, \quad g_1(t) = -\frac{e^{-\frac{1}{t}}}{t^{3/2}}\left(1 - \frac{2}{t}\right) \tag{45}$$

$$f_{2\beta}(t) = \frac{3\,g_2\left(t/\beta^2\right)}{2\sqrt{\pi}\,\beta^4}, \quad g_2(t) = -\frac{e^{-\frac{1}{t}}}{t^{5/2}}\left(1 - \frac{2}{3t}\right) \tag{46}$$

$$f_{3\beta}(t) = \frac{3\,g_3\left(t/\beta^2\right)}{4\sqrt{\pi}\,\beta^5}, \quad g_3(t) = \frac{e^{-\frac{1}{t}}}{t^{5/2}}\left(1 - \frac{4}{t} + \frac{4}{3t^2}\right) \tag{47}$$

$$f_{4\beta}(t) = \frac{15\,g_4\left(t/\beta^2\right)}{4\sqrt{\pi}\,\beta^6}, \quad g_4(t) = \frac{e^{-\frac{1}{t}}}{t^{7/2}}\left(1 - \frac{4}{3t} + \frac{4}{15t^2}\right) \tag{48}$$

$$f_{5\beta}(t) = \frac{15\,g_5\left(t/\beta^2\right)}{8\sqrt{\pi}\,\beta^7}, \quad g_5(t) = -\frac{e^{-\frac{1}{t}}}{t^{7/2}}\left(1 - \frac{6}{t} + \frac{4}{t^2} - \frac{8}{15t^3}\right) \tag{49}$$

$$f_{6\beta}(t) = \frac{105\,g_6\left(t/\beta^2\right)}{8\sqrt{\pi}\,\beta^8}, \quad g_6(t) = -\frac{e^{-\frac{1}{t}}}{t^{9/2}}\left(1 - \frac{2}{t} + \frac{4}{5t^2} - \frac{8}{105t^3}\right) \tag{50}$$

For practical reasons higher values of $\alpha$ are not necessarily due to the limitation of shell filling with electrons.

## C. QUADRATURE FORMULA FOR THE LAPLACE INTEGRAL

To obtain the decomposition (8) for given $\alpha$ and $\beta$ we make a substitution $s \to s^2$ into the equation (10)

$$F_{\alpha\beta}(s^2) = s^\alpha e^{-2\beta s} = \int_0^\infty e^{-s^2 x} f_{\alpha\beta}(x)\,dx, \tag{51}$$

then introduce another variable $x = e^t$ in the integral

$$F_{\alpha\beta}(s^2) = s^\alpha e^{-2\beta s} = \int_{-\infty}^\infty e^{-s^2 e^t + t} f_{\alpha\beta}(e^t) dt. \tag{52}$$

The function under the integral (52) has exponential decay both in the spatial and frequency domains. Therefore the truncated trapezoidal rule gives the optimal convergence rate. It turns out to the final approximation of the form

$$F_{\alpha\beta}(s^2) \approx \sum_{k=0}^{K} w_k e^{t_k} f_{\alpha\beta}(e^{t_k}) e^{-s^2 e^{t_k}} \tag{53}$$

with trapezoidal weights $w_k$ and the integrand values in the nodes $e^{-s^2 e^{t_k} + t_k} f_{\alpha\beta}(e^{t_k})$. The Gaussian-like part is split out in a separate factor in correspondence with decomposition (8). Parameters of the formula

$$t_k = a_t + k h_t, \quad h_t = (b_t - a_t)/K \tag{54}$$

have to be selected in such a way that the resulting quadrature formula approximates the integral for a wide range of parameter $s$. Typically, the choice $a_t \gtrsim -3$, $b_t \lesssim 45$, and $K \sim 250$ gives good accuracy ($\leq 10^{-7}$). As an example, in Table II the required number of terms in sum (53) is presented. Accurate error analysis can be found in [34].



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## D. CONVERGENCE RATE OF $K(N)$ FOR THE SLATER DENSITY SERIES

In this section we estimate an upper bound $K$ in sum (11) which has the logarithmic dependence on the mesh size $N$. We follow the proof given in paper [47] for Lemma 4.3. In this Lemma a Slater-type function $\rho(\sqrt{s})$ from eq. (10) is considered for $\alpha = 0$. Below, this function is considered for integer $\alpha$.

The integrand in (10) after the change of variables $t = e^x$

$$P_{\alpha\beta}(x) = e^{-se^x + x} f_{\alpha\beta}(e^x) \tag{55}$$

has the following decay on the real axis (skipping the numerical factor before the exponent)

$$P_{\alpha\beta}(x) \approx e^{-se^x - c_1 x}, \quad \text{as } x \to \infty, \quad c_1 = \frac{\alpha + 1 - (\alpha \bmod 2)}{2}, \tag{56}$$

$$P_{\alpha\beta}(x) \approx e^{-\beta^2 e^{|x|} + c_2 |x|}, \quad \text{as } x \to -\infty, \quad c_2 = \alpha + \frac{1}{2}. \tag{57}$$

This immediately implies expression (5.3) from [47] for $b = \min(\beta^2, s)$, $b$ is taken in the notation of [47]. Following then the statement I of Lemma 4.3 we may conclude, that $K = \mathcal{O}(|\log\varepsilon|(|\log\varepsilon| + \log 1/b))$ with the error $\varepsilon$ of the approximation and $b \sim 1/N^2$.

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